

The Fokker-Planck equation for bistable potential in the optimized expansion

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Abstract

The optimized expansion is used to formulate a systematic approximation scheme to the probability distribution of a stochastic system. The first order approximation for the one-dimensional system driven by noise in an anharmonic potential is shown to agree well with the exact solution of the Fokker-Planck equation. Even for a bistable system the whole period of evolution to equilibrium is correctly described at various noise intensities.

1 Introduction

The Fokker-Planck (FP) equation is widely used to describe non-equilibrium systems in physics, chemistry and biology [1]. The stochastic approach consists in representing the most relevant degrees of freedom of the system by the variable x driven by noise and deterministic interaction potential $U(x, t)$. The time development of the probability distribution $W(x, t)$ is given by a

partial differential equation

$$\frac{\partial}{\partial t}W(x, t) = \mathbf{L}_{\text{FP}}\mathbf{W}(\mathbf{x}, \mathbf{t}) := \frac{\partial}{\partial \mathbf{x}}[\mathbf{U}'(\mathbf{x}, \mathbf{t})\mathbf{W}(\mathbf{x}, \mathbf{t}) + \mathbf{D}\frac{\partial^2}{\partial \mathbf{x}^2}\mathbf{W}(\mathbf{x}, \mathbf{t}) \quad (1)$$

where the diffusion coefficient, D , represents a noise intensity and $U'(x, t)$, denoting the derivative of the interaction potential with respect to x , is called the drift coefficient. The Green's function of the FP equation, $P(x, t|x', t')$ which fulfils the initial condition $P(x, t|x', t') = \delta(x, x')$, is called the transition probability (conditional probability), since it describes the evolution of the probability density from time t' to t :

$$W(x, t) = \int P(x, t|x', t')W(x', t')dx'. \quad (2)$$

For a time independent potential, $U(x)$, the separation ansatz

$$W(x, t) = \Phi(x)e^{-\kappa t} \quad (3)$$

reduces the time dependent FP equation(1) to the stationary eigenfunction equation

$$\mathbf{L}_{\text{FP}}\Phi(\mathbf{x}) = \frac{\partial \mathbf{U}'(\mathbf{x})\Phi(\mathbf{x})}{\partial \mathbf{x}} + \mathbf{D}\frac{\partial^2 \Phi(\mathbf{x})}{\partial \mathbf{x}^2} = -\kappa\Phi(\mathbf{x}). \quad (4)$$

The lowest eigenvalue of a FP operator is identically zero, $\kappa = 0$, and the corresponding eigenfunction $\Phi_0(x)$ can be found exactly, yielding the stationary probability distribution of the form

$$W_{st}(x) = \Phi_0(x) = Ne^{-\frac{U(x)}{D}} \quad (5)$$

with the normalization constant $N = (\int_{-\infty}^{\infty} e^{-\frac{U(x)}{D}} dx)^{-1}$. For an arbitrary potential $U(x)$ the higher eigenfunctions and the non-stationary probability distribution cannot be found exactly, there is thus a need to develop approximation methods. To this end it is convenient to transform the FP equation into the Schrödinger equation [1]. The transformation

$$\Psi(x) = e^{\frac{U(x)}{2D}}\Phi(x) \quad (6)$$

brings the FP operator to the Hermitian form

$$\mathcal{L} = e^{\frac{U(x)}{2D}}L_{\text{FP}}e^{-\frac{U(x)}{2D}} = D\frac{d^2}{dx^2} - V(x) \quad (7)$$

where

$$V(x) = \frac{[U'(x)]^2}{4D} - \frac{U''(x)}{2}. \quad (8)$$

The operator $\hbar\mathcal{L}$ has the same form as the negative Hamiltonian operator for the quantum mechanical particle of the mass $M = \frac{\hbar}{2D}$ in the potential $\hbar V(x)$. The transformed FP equation

$$\mathcal{L}\Psi(x) = \left(D \frac{d^2}{dx^2} - V(x) \right) \Psi(x) = \lambda \Psi(x) \quad (9)$$

is called a pseudo-Schrödinger equation, because by (3) the wave function, Ψ , evolves in imaginary time $t_S = -i\hbar t$. The transition probability, $P(x, t|x', t')$, being the Green's function of the original FP equation (1), is related to the imaginary time evolution amplitude, $K(x, t; x', t')$, of the pseudo-Schrödinger equation (9) by

$$P(x, t|x', t') = \exp\left(\frac{U(x') - U(x)}{2D}\right) K(x, t; x', t'). \quad (10)$$

The evolution amplitude can be represented as a path integral

$$K(x, t|x', t') = \int_{x(t')=x'}^{x(t)=x} Dx e^{-\int_{t'}^t L[x] dt} \quad (11)$$

over all functions which begin at $x(t') = x'$ and end at $x(t) = x$, where the pseudo-Schrödinger Lagrangian of a particle is given by

$$L[x] = \frac{\dot{x}^2}{4D} + V(x). \quad (12)$$

We shall study a stochastic system in an anharmonic potential,

$$U(x) = \frac{\gamma x^2}{2} + \lambda x^4. \quad (13)$$

In this case the pseudo-Schrödinger potential (8) takes the form:

$$V(x) = -\frac{\gamma}{2} + \left(\frac{\gamma^2}{4D} - 6\lambda \right) x^2 + \frac{2\lambda\gamma}{D} x^4 + 4\frac{\lambda^2 x^6}{D}. \quad (14)$$

For vanishing λ the problem reduces to the exactly solvable Ornstein-Uhlenbeck process in a quadratic interaction potential, $U(x) = \frac{\gamma x^2}{2}$. In this case the pseudo-Schrödinger potential is also quadratic, $V(x) = -\frac{\gamma}{2} + \frac{\gamma^2}{4D}x^2$, and the path integral for the evolution amplitude (11) can be performed exactly yielding

$$K_\gamma(x, t|x', t') = \sqrt{\frac{\gamma}{2\pi D(1 - e^{-2\gamma(t-t')})}} \times \exp \left\{ \frac{\gamma}{4D \sinh(\gamma(t-t'))} [(x^2 + x'^2) \cosh(\gamma(t-t')) - 2xx'] \right\}. \quad (15)$$

By (2) this leads to an exact expression for the transition probability of the Ornstein-Uhlenbeck process

$$P_\gamma(x, t|x', t') = \sqrt{\frac{\gamma}{2\pi D(1 - e^{-2\gamma(t-t')})}} \exp \left(-\frac{\gamma(x - x'e^{-\gamma(t-t')})^2}{2D(1 - e^{-2\gamma(t-t')})} \right). \quad (16)$$

In the presence of anharmonicity ($\lambda \neq 0$) the evolution amplitude, $K(x, t; x', t')$, cannot be obtained exactly, but various approximation methods are developed. The perturbative calculations of $P(x, t|x', t')$ in powers of λ are possible if $\gamma > 0$. In this case the first order approximation describes well the evolution of the system approaching the stationary distribution in the long time limit, only the normalization worsens with increasing λ . However, for $\gamma < 0$ the method becomes inapplicable, since the transition probability is non-normalizable. In this case the perturbative approximations give a wrong description of the time evolution, since the maxima of the transition probability escape to $x = \pm\infty$.

Few years ago we proposed the optimized expansion (OE) scheme for the evolution amplitude [2] which has much better convergence properties than the perturbative expansion in powers of λ . Here we apply this method to generate a systematic approximation scheme for the transition amplitude $P(x, t|x', t')$ by (2). We will show that the method can be successfully applied for describing the time evolution of a stochastic systems. The efficiency of the method will be shown on the example of bistable system driven by noise in the double-well potential. Such a system attracts much attention in nonlinear optics (statistical properties of laser light above threshold), solid-state physics and chemistry. The solution of the FP equation which describes the

evolution from an intrinsically unstable state to the final stationary state is of a special interest, and various approximation methods have been proposed and compared with the numerical solution in this case. However, in all the methods the evolution process is divided into few steps and different approximations are used in each time sector [3]. We will show that the first order result of the OE provides a simple approximation which agrees well with the exact solution of the FP equation in the whole period of evolution to equilibrium at various noise intensities.

2 The optimized expansion

The optimized expansion (OE) has been formulated as a method to generate non-perturbative approximations for the effective action in quantum field theory [4]. The method consists in calculating the effective action as a series in ϵ , by splitting the Lagrangian into

$$L = L_0 + \epsilon(L - L_0), \quad (17)$$

where the unperturbed part contains arbitrary parameters, which are optimized in every order calculation (upon setting $\epsilon = 1$). The method is equivalent to a systematic re-summation of the perturbation series and gives the Hartree-Fock-Bogolubov approximation in the leading order. A similar idea has been applied to formulate systematic approximation methods for other physical quantities in a number of works [5, 6] under different names (self-similar perturbation theory, delta expansion, variational perturbation theory, optimized perturbation theory...). The approach provides a method to systematically improve any self-consistent approximation of the theory. The OE has been also applied to the quantum mechanics of the particle in the potential $V(x)$ by modifying the classical Lagrangian to the form

$$L[x] = L_\omega + \epsilon V_{int} = \frac{M\dot{x}^2}{2} + \frac{M\omega^2 x^2}{2} + \epsilon \left(V(x) - \frac{M\omega^2 x^2}{2} \right), \quad (18)$$

where the harmonic oscillator of the mass M and an arbitrary frequency ω is chosen as the unperturbed system, and calculating physical quantities as a series in powers of ϵ . It has been shown, that for the ground state energy of the quantum mechanical anharmonic oscillator a convergent series

is obtained [7, 6], as opposed to perturbative series which is asymptotic. Applying the method to calculate the imaginary time evolution amplitude [2, 8], it is convenient to represent the series for $W(x, t; x', t') = \ln K(x, t; x' t')$ by the cumulant expansion. For the particle of the mass $\frac{\hbar}{2D}$ we have

$$\begin{aligned} W(x, t; x', t') &= W_\omega(x, t; x', t') - \epsilon \langle V_{int}(x) \rangle_\omega \\ &+ \frac{\epsilon^2}{2} (\langle V_{int}^2(x) \rangle_\omega - \langle V_{int}(x) \rangle_\omega \langle V_{int}(x) \rangle_\omega) - \dots \end{aligned} \quad (19)$$

where by (15)

$$\begin{aligned} W_\omega(x, x', t, t') &= \ln K_\omega(x, x', t, t') = \\ &\frac{1}{2} \ln \left(\frac{\omega}{4\pi D \sinh \omega(t - t')} \right) - \frac{\omega [(x^2 + x'^2) \cosh \omega(t - t') - 2xx']}{4D \sinh \omega(t - t')} \end{aligned} \quad (20)$$

and the expectation values are calculated for the unperturbed Lagrangian

$$\langle \dots \rangle_\omega = \int_{x(t')=x'}^{x(t)=x} Dx \dots e^{-\int_{t'}^t L_\omega[x] dt}. \quad (21)$$

The N -th order approximant, $W^{(N)}(x' t'; x, t)$, is obtained by truncating the series (19) after the N -th term and setting $\epsilon = 1$, since only in this case does the modified action agree with the classical one. The exact result, being a sum of an infinite series, would not depend on arbitrary frequency, but any finite order truncation shows such a dependence. We choose, therefore, the value of the unperturbed frequency, ω , to make the given order approximant as insensitive as possible to its small variation, by requiring

$$\frac{\delta W^{(N)}}{\delta \omega} = 0. \quad (22)$$

The optimization condition determines the value of ω as a function of β, x and x' , which changes from order to order, improving the convergence properties of the approximation scheme.

In the case of polynomial potential the expectation values in $W^{(N)}$ (19) are given by Gaussian functional integrals which can be easily performed, yielding an analytic expression for $W^{(N)}$. The first order result for the evolution amplitude of the quartic oscillator has been obtained in Ref. [2], and shown to give a satisfactory approximation to the particle density in the

broad range of the oscillator parameters. Here we have to calculate the evolution amplitude in the potential

$$V(x) = g_0 + g_2x^2 + g_4x^4 + g_6x^6, \quad (23)$$

because the pseudo-Schrödinger potential corresponding to the bistable FP equation (14) is sextic. After setting $\epsilon = 1$ the first order results can be written as

$$\begin{aligned} W^{(1)}(x, t; x', t') = & -tg_0 + W_\omega(x, t; x', t') + \left(\frac{\omega^2}{2} - g_2\right) \int_{t'}^t [L^2(\tau) + K(\tau)] d\tau \\ & - g_4 \int_{t'}^t [L^4(\tau) + 6L^2(\tau)K(\tau) + 3K^2(\tau)] d\tau \\ & - g_6 \int_{t'}^t [L^6(\tau) + 15K(\tau)L^4(\tau) + 45K^2(\tau)L^2(\tau) + 15K^3(\tau)] d\tau \end{aligned} \quad (24)$$

where

$$L(\tau) = \frac{x \sinh \omega(\tau - t') + x_b \sinh \omega(t - \tau)}{\sinh \omega(t - t')} \text{ and } K(\tau) = \frac{2D \sinh \omega(\tau - t') \sinh \omega(t - \tau)}{\omega \sinh \omega(t - t')}$$

and the optimization condition (22) reduces to

$$\begin{aligned} \left(g_2 - \frac{\omega^2}{2}\right) \frac{\partial}{\partial \omega^2} \int_{t'}^t [L^2(\tau) + K(\tau)] d\tau + g_4 \frac{\partial}{\partial \omega^2} \int_{t'}^t [L^4(\tau) + 6L^2(\tau)K(\tau) + 3K^2(\tau)] d\tau \\ + g_6 \frac{\partial}{\partial \omega^2} \int_{t'}^t [L^6(\tau) + 15K(\tau)L^4(\tau) + 45K^2(\tau)L^2(\tau) + 15K^3(\tau)] d\tau = 0. \end{aligned} \quad (25)$$

Upon performing the integrals in the above expressions an analytic expression for the evolution amplitude $K(x, t|x', t') = e^{W(x, t; x', t')}$ is obtained. The result is optimized by choosing the value of the frequency to fulfil (25) and used to calculate the first order approximation to the transition probability $P(x, t|x', t')$ according to Eq.2.

After completing this work we learned that approximate solutions of the FP equation in an anharmonic potential have been also studied by directly improving the perturbative expansion of the transition probability, using a drift coefficient as a variational parameter [9]. The variational expressions substantially differ from ours, because the sextic term of the pseudo-Schrödinger potential (14) does not contribute to the first order in their method. The numerical results are also different, especially in the case of the bistable potential.

3 Results and conclusions

The approximation obtained in the first order of the OE is exact at $\lambda = 0$, and it gives very good results when the anharmonic terms are small and the pseudo-Schrödinger potential is convex ($\gamma > 0$). The shape of the transition probability is well described, but the total probability slowly decreases in time. A similar problem appears in the first order calculation in the variational perturbation method [9], where the total probability increases in time. The spoiling of the normalization by optimization is a general feature of perturbative schemes with variational parameters [10] and can be cured by normalizing the each order result by hand. The normalized probability distribution obtained in the first order of the OE shows a good agreement with the exact solution of the FP equation in the whole period of evolution. Here we show the results in the most demanding case of double-well interaction potential ($\gamma < 0$), when the pseudo-Schrödinger potential has a multiple-well structure. The critical value of the diffusion coefficient ($D_{cr} = \frac{\gamma^2}{24\lambda}$), distinguishes two cases: the pseudo-Schrödinger potential of double-well shape in the case of large noise ($D > D_{cr}$), and of triple-well shape in the case of small noise.

We compare the results of our approximation to the transition probability, $P(x, t|0, 0)$, with the exact results calculated numerically in Ref. [3] and Ref. [11] for the interaction potential $U(x) = -\frac{1}{2}x^2 + \frac{1}{4}x^4$, which corresponds to $\gamma = -1$ and $\lambda = \frac{1}{4}$ in our notation. The critical value of the diffusion coefficient is $D_{cr} = \frac{1}{6}$ in this case. The results for the time evolution of the transition probability at noise intensity $D = 0.1$ are shown in Fig.1, and the results at $D = 0.05$ and $D = 0.01$, in Fig.2 and Fig.3, respectively. The pseudo-Schrödinger potential for the considered values of D is also plotted.

The transition probability for the system being initially in the unstable state ($P(x, 0|0, 0) = \delta(x - 0)$) is presented at different times of the evolution: the first value is in the initial time region, the next ones are in the intermediary region, and the last one is in the final time region when the stationary distribution is already achieved. It is remarkable that a good description of the evolution from the unstable configuration to the stable one is obtained already in the first order of the OE, even in the difficult case of small noise. This is due to the optimization of the variational parameter ω at a given point x in the considered time t . One has to stress, that in our calculation the stationarity condition, which determines the optimal value

of ω (25), has a solution for all the values of x during the whole period of evolution. This is in difference with the variational perturbation method [9], where different criteria of the variational parameter fixing are used in the initial and in the final regions, and the worst description is obtained in the intermediate stage of evolution. In our approximation the initial and intermediate stage of evolution are described very well for all values of noise, but the discrepancies appear in the final stage of evolution and the asymptotic distribution differs from the exact one. For $D = 0.05$ and $D = 0.01$ the approximation is of similar quality as the two or three-stage approximations based on Ω expansion [3], and gives also a good description for $D = 0.1$, when the approximation discussed by Hu becomes inaccurate as observed in Ref. [11]. The accuracy of our approximation can be improved by higher order calculation in a systematic way.

One has to note that an extension of this approach to higher dimensional systems is possible. Also the dynamics of a bistable stochastic system driven by time-dependent forces can be studied in the OE. The influence of a periodic force on the bistable system, which is a topic of current interest because of the phenomenon of stochastic resonance, will be discussed in a future publication.

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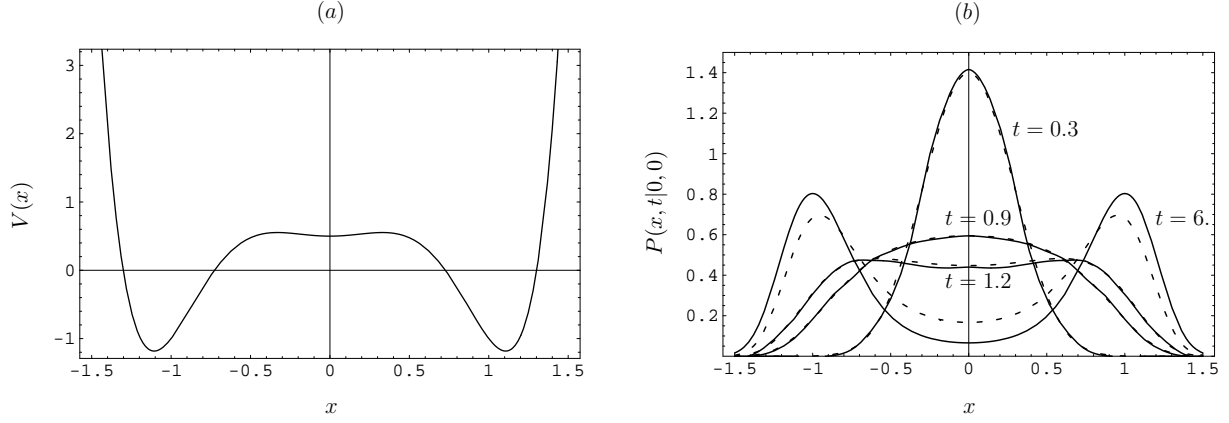


Figure 1: The pseudo-Schrödinger potential (a) and the time evolution of $P(x, t|0, 0)$ (b) for the bistable potential $U(x) = -\frac{x^2}{2} + x^4$ at $D = 0.1$ in the first order of the OE (*dashed line*) at $t = 0.3$, $t = 0.9$, $t = 1.2$ and $t = 6.$, compared with the exact results taken from Ref. [11] (*solid line*)

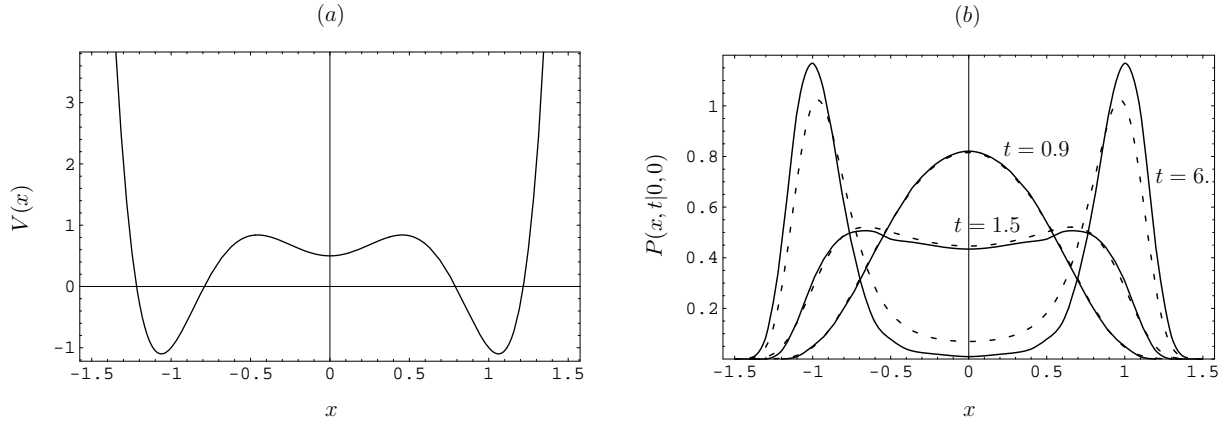


Figure 2: Same as in Fig.1, but for $D = 0.05$. at the time $t = 0.9$, $t = 1.5$ and $t = 6.$, compared with the exact results taken from Ref. [3] (*solid line*).

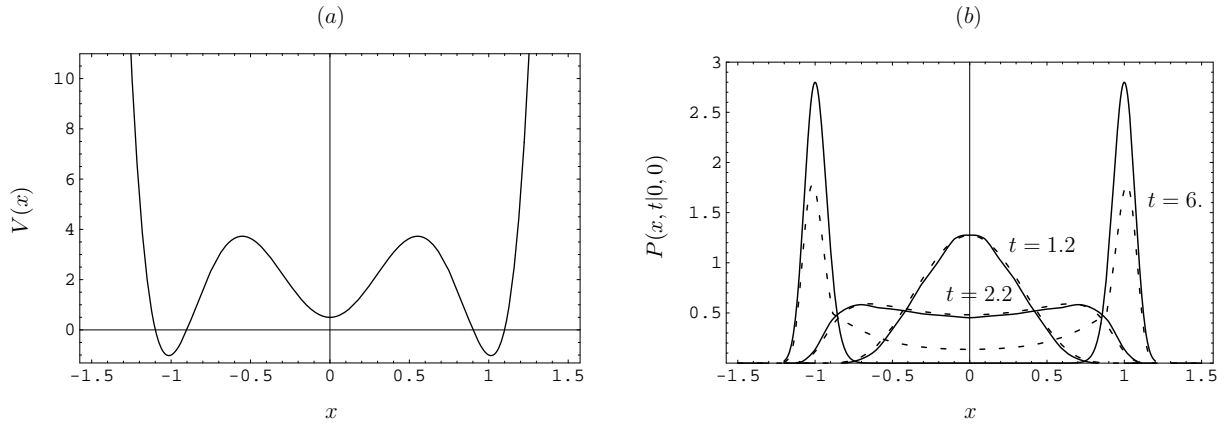


Figure 3: Same as in Fig.1, but for $D = 0.01$. at the time $t = 1.2$, $t = 2.2$ and $t = 6.1$, compared with the exact results taken from Ref. [3] (solid line).